An algorithm for computing cutpoints in finite metric spaces

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Abstract

The theory of the *tight span*, a cell complex that can be associated to every metric D, offers a unifying view on existing approaches for analyzing distance data, in particular for decomposing a metric D into a sum of simpler metrics as well as for representing it by certain specific edge-weighted graphs, often referred to as *realizations* of D. Many of these approaches involve the explicit or implicit computation of the so-called cutpoints of (the tight span of) D, such as the algorithm for computing the "building blocks" of optimal realizations of D recently presented by A.Hertz and S.Varone. The main result of this paper is an algorithm for computing the set of these cutpoints for a metric D on a finite set with n elements in $O(n^3)$ time. As a direct consequence, this improves the run time of the aforementioned $O(n^6)$-algorithm by Hertz and Varone by "three orders of magnitude".

Keywords: metric, cutpoint, realization, tight span, decomposition, block

1 Introduction

The decomposition of a given metric into simpler metrics (see e.g. [5]) is a fundamental problem in classification featuring applications in, for example, clustering (e.g. [2]), "networking" (e.g. [3]), and phylogenetics (e.g. [15]). The theory of the *tight span*

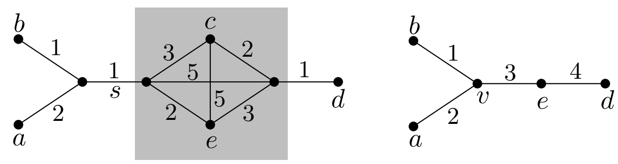
$$T(D) := \{f \in \mathbb{R}^X : f(x) = \sup_{y \in X}\big(D(x,y) - f(y)\big) \text{ for all } x \in X\},$$

of a metric D defined on a set X [17, 6] offers a unifying view on various existing approaches developed for this task. In this paper, we focus on decompositions of metrics D defined on a finite set X that are induced by *cutpoints* of $T(D)$, that is, maps $f \in T(D)$ such that $T(D) - \{f\}$ is disconnected. These decompositions are closely related to certain *graph realizations* of D, that is, connected edge-weighted graphs $G = (V, E, \ell : E \to \mathbb{R}_{>0})$ with $X \subseteq V$ for which $D(x,y) = D_G(x,y)$ holds for all $x, y \in X$ (where D_G denotes the shortest-path metric induced by G on V).

To describe these graph realizations, recall (see e.g. [20]) that a vertex v in a graph $G = (V, E)$ is called a *cut vertex* (of G) if there exist vertices $u, u' \in V$ with $\{u, v\}, \{u', v\} \in E$ such that every path from u to u' in G passes through v. Moreover, a maximal subset $B \subseteq V$ with the property that

D	a	b	c	d	e
a	0	3	6	9	5
b	3	0	5	8	4
c	6	5	0	3	5
d	9	8	3	0	4
e	5	4	5	4	0

(a)



(b) (c)

Figure 1: (a) An example of a metric D on $X = \{a, \ldots, e\}$. (b) A block realization of D: The vertices in the shaded region form a block and edge s is a bridge. (c) A block realization of the restriction D' of D to the subset $X' := X \setminus \{c\}$.

the induced graph $G[B] := (B, E \cap \binom{B}{2})$ has no cut vertex is called a *block* of G. A graph realization G of D is called a *block realization* of D if G is a *block graph*, i.e., every block of G is a clique, and every vertex in $V \setminus X$ has degree at least 3 and is a cut vertex of G. An example of a block realization is presented in Figure 1(b).

In a recent series of papers [8, 9, 10], it has been observed that a map $f \in T(D)$ is a cutpoint if and only if the graph $\Gamma_f := (X_f, E_f)$ defined, for every $f \in \mathbb{R}^X$, by $X_f := \mathrm{supp}(f)$ and $E_f := \big\{\{x, y\} \in \binom{\mathrm{supp}(f)}{2} : f(x) + f(y) > D(x, y)\big\}$ is disconnected (where, as usual, $\mathrm{supp}(f) := \{x \in X : f(x) \neq 0\}$ denotes the *support* of f), that a map f in

$$P(D) := \{f \in \mathbb{R}^X : f(x) + f(y) \geq D(x, y) \text{ for all } x \in X\}$$

for which the graph Γ_f is disconnected must be contained in — and, hence, a cutpoint of — $T(D)$, and that a cutpoint $f \in T(D)$ has a neighborhood that is homeomorphic to the open interval $(-1, +1)$ if and only if Γ_f is the disjoint union of two cliques. As such maps are of little interest for constructing block realizations, we will focus our attention in particular to the set of those cutpoints, denoted by $cut^*(D)$, for which either $\mathrm{supp}(f) \neq X$ holds or Γ_f is not the disjoint union of two cliques.

In this paper, we present an algorithm with run time $O(n^3)$ to compute $cut^*(D)$, where $n = |X|$, improving the run time of the algorithm presented in [7]. Once the set $cut^*(D)$ is available, it is straight-forward to compute a corresponding canonical block realization $G = G_D = (V_D, E_D, \ell_D)$ of D in $O(n^3)$ time. And, from that block realization it is then easy to derive, for every block B of G_D, a corresponding metric D_B on X that assigns, to any two elements $x, x' \in X$, the value $D_B(x, x')$ defined as the total weight of

those edges on any shortest path from x to x' in G that have both end points in B. For example in Figure 1(b) the distance $D_B(a, d)$ between a and d is 5 where B is the block in the shaded region.

This yields a decomposition of D into a sum of metrics of the form D_B where B runs through the blocks of G_D that can be computed in $O(n^3)$ time. As a consequence, our algorithm improves the run time of the algorithm presented in [14] that follows a 2-step approach: It computes first those metrics D_B that correspond to blocks B with only 2 vertices, the so-called *bridges*, (see [13] for details) and then the remaining metrics D_B for the blocks B that are not bridges.

Our paper is structured as follows. In the next section, we introduce the concept of block splits and show how they can help in the computation of $cut^*(D)$. In Section 3, we establish the key properties of block splits and cutpoints in $cut^*(D)$ that we use in our new algorithm for computing $cut^*(D)$, and we present this algorithm in Section 4.

2 Block splits

In this section, we present a key concept used in our algorithm for computing the set $cut^*(D)$, where D is the given metric on a finite set X: Recall that a *split* S of X is a bipartition of X into two non-empty subsets A and B, also denoted by $A|B$ or $B|A$. A split $A|B$ of X is called a *block split* of X (relative to D) if there exists a map $f \in P(D)$ with $\mathrm{supp}(f) = X$ such that Γ_f is the disjoint union of two cliques whose vertex sets are A and B, respectively. Note that the condition used in the definition of a block split above is slightly stronger than the condition given in [16, p. 10]. Also note that block splits, although not given a specific name, play an important role in the algorithm for computing bridges presented in [13]. The set of block splits of X induced by D is denoted by Σ_D. In the following, we will also often simply write xy for $D(x, y)$, $x, y \in X$.

Our first goal is to establish a property of block splits that allows to efficiently check whether a given split of X is a block split. To this end, we first recall the following well-known fact.

Lemma 2.1 Given two sets A and B and a bi-variate map $\phi : A \times B \to \mathbb{R}$ from the Cartesian product $A \times B$ into the real numbers (or any Abelian group), there exist maps $\phi_A : A \to \mathbb{R}$ and $\phi_B : B \to \mathbb{R}$ with $\phi(a, b) = \phi_A(a)+$

$\phi_B(b)$ for all $a \in A$ and $b \in B$ if and only if $\phi(a,b)+\phi(a',b') = \phi(a,b')+\phi(a',b)$ holds for all $a, a' \in A$ and $b, b' \in B$ if and only if $\phi(a,b) + \phi(a_0,b_0) = \phi(a,b_0) + \phi(a_0,b)$ holds for some fixed elements $a_0 \in A$ and $b_0 \in B$ and all $a \in A$ and $b \in B$.

Proof: If there exist maps $\phi_A : A \to \mathbb{R}$ and $\phi_B : B \to \mathbb{R}$ with $\phi(a,b) = \phi_A(a) + \phi_B(b)$, one clearly has $\phi(a,b) + \phi(a',b') = \phi_A(a) + \phi_B(b) + \phi_A(a') + \phi_B(b') = \phi(a,b') + \phi(a',b)$ for all $a, a' \in A$ and $b, b' \in B$ while, conversely, if $\phi(a,b) + \phi(a_0,b_0) = \phi(a,b_0) + \phi(a_0,b)$ holds for some fixed elements $a_0 \in A$ and $b_0 \in B$ and all $a \in A$ and $b \in B$, one has $\phi(a,b) = \phi_A(a) + \phi_B(b)$ for, e.g., the two maps $\phi_A : A \to \mathbb{R} : a \mapsto \phi(a,b_0)$ and $\phi_B : B \to \mathbb{R} : b \mapsto \phi(a_0,b) - \phi(a_0,b_0)$. ■

Next, we define, for any map $f \in P(D)$ and any subset Y of X, the *virtual distance* $D(f|Y)$ from f to Y (relative to D) by

$$D(f|Y) := \frac{1}{2}\min\{f(y) + f(y') - yy' : y, y' \in Y\}.$$

We will also write $D(x|Y)$ rather that $D(f|Y)$ in case f coincides with the so-called *Kuratowski map* k_x [18] associated with an element $x \in X$ defined by $k_x(y) := xy$ for all $y \in X$. Note that $0 \leq D(f|Y)$ holds for all f and Y as above. Note also that, given a split $S = A|B$ of X with $ab + a'b' = ab' + a'b$ for all $a, a' \in A$ and $b, b' \in B$, and any two elements $a \in A$ and $b \in B$, one has

$$\begin{aligned}
& D(a|B) + D(b|A) - ab \qquad (1)\\
&= \frac{1}{2}\min_{a',a''\in A; b',b''\in B}\{ab' + ab'' + a'b + a''b - b'b'' - a'a'' - 2ab\}\\
&= \frac{1}{2}\min_{a',a''\in A; b',b''\in B}\{a'b' + a''b'' - b'b'' - a'a''\}\\
&= \frac{1}{2}\min_{a',a''\in A; b',b''\in B}\{\max(a'b' + a''b'', a'b'' + a''b') - a'a'' - b'b''\} =: \alpha_S,
\end{aligned}$$

and that α_S has been dubbed the *isolation index* of S [1].

To illustrate the above definitions, note that, for the metric given in Figure 1(a), the split $S = \{a,b\}|\{c,d,e\}$ is a block split with $D(a|\{c,d,e\}) = 3$, $D(b|\{c,d,e\}) = 2$, $D(c|\{a,b\}) = 4$, $D(d|\{a,b\}) = 7$, and $D(e|\{a,b\}) = 3$ and, therefore, $D(x|\{c,d,e\}) + D(y|\{a,b\}) - D(x,y) = 1$, for all $x \in \{a,b\}$

and $y \in \{c, d, e\}$, the weight of the edge s separating $\{a, b\}$ from $\{c, d, e\}$ in the corresponding block realization depicted in Figure 1(b).

More generally, we have

Lemma 2.2 A split $S = A|B$ of X is a block split of X if and only if the isolation index α_S of S is positive and, choosing arbitrary elements $a_0 \in A$ and $b_0 \in B$, $a_0 b_0 + a'b' = a_0 b' + a'b_0$ holds for all $a' \in A$ and $b' \in B$.

Proof: Assume first that $S = A|B$ is a block split. By the definition of a block split, there exists a map $f \in P(D)$ for which Γ_f is the disjoint union of two cliques whose vertex sets are A and B and, therefore, we clearly have $D(f|A), D(f|B) > 0$. Moreover, for the restrictions $\phi_A := f|_A$ and $\phi_B := f|_B$ of f to A and B, respectively, we have $\phi_A(a) + \phi_B(b) = ab$ for all $a \in A$ and $b \in B$, and, therefore, $ab + a'b' = ab' + a'b$ must hold for all $a, a' \in A$ and $b, b' \in B$ in view of Lemma 2.1 applied to the bivariate map $\phi := D|_{A\times B}$. In consequence, by Equation (1), we have $D(a|B) + D(b|A) - ab = \alpha_S$ for all $a \in A$, $b \in B$ and, so, choosing any $a \in A$ and $b \in B$, we also have

$$\begin{aligned}
\alpha_S &= D(a|B) + D(b|A) - ab \\
&= \frac{1}{2} \min_{a',a''\in A; b',b''\in B} \{f(b') + f(b'') - b'b'' + f(a') + f(a'') - a'a''\} \\
&= D(f|B) + D(f|A) > 0 \text{ , as required.}
\end{aligned}$$

Conversely, choosing arbitrary elements $a_0 \in A$ and $b_0 \in B$, if $a_0 b_0 + a'b' = a_0 b' + a'b_0$ holds for all $a' \in A$ and $b' \in B$ and the isolation index of S is positive, then, in view of Lemma 2.1, we may choose any two non-negative real numbers γ_A, γ_B with $\gamma_A + \gamma_B = \alpha_S$ and define the map

$$f = f_{A\to\gamma_A, B\to\gamma_B} : X \to \mathbb{R} \tag{2}$$

by $f(a) := D(a|B) - \gamma_A$ for all $a \in A$ and $f(b) := D(b|A) - \gamma_B$ for all $b \in B$. In view of Equation (1), we clearly have $f(a) + f(b) = D(a|B) + D(b|A) - \alpha_S = ab$ for all $a \in A$ and $b \in B$. Moreover, we have $f(a) + f(a') \geq aa'$ for all $a, a' \in A$ as $f(a) + f(a') \geq D(a|B) + D(a'|B) - 2\alpha_S = ab + a'b - 2D(b|A) = aa' + (ab + a'b - aa') - 2D(b|A) \geq aa'$ holds for all $a, a' \in A$ and every $b \in B$ in view of the definition of $D(b|A)$ $\big($indeed, $ab + a'b - aa'$ is one of the terms whose minimum, over all $a, a' \in A$, coincides with $2D(b|A)\big)$, and we have $f(a) + f(a') > aa'$ for all $a, a' \in A$ if and only $\gamma_A < \alpha_S$ holds as $\gamma_A = \alpha_S$ implies $f(a) + f(a') = aa'$ for all $a, a' \in A$ with $ab + a'b - aa' = 2D(b|A)$. By

symmetry, we have also $f(b)+f(b') \geq bb'$ for all $b, b' \in B$ and $f(b)+f(b') > bb'$ if and only if $\gamma_B < \alpha_S$ holds. Thus, E_f is a subset of $\binom{A}{2} \cup \binom{B}{2}$, and it coincides with this set if and only if $\gamma_A, \gamma_B < \alpha_S$ holds. So, $A|B$ must indeed be a block split, as required. ■

It is also worth noting that, for every block split $S = A|B$, every $f \in P(D)$ with $E_f \subseteq \binom{A}{2} \cup \binom{B}{2}$ (or, equivalently, with $f(a) + f(b) = ab$ for all $a \in A$ and $b \in B$) actually is of the form $f = f_{A\to\gamma_A,B\to\gamma_B}$ for some $\gamma_A, \gamma_B \geq 0$ with $\gamma_A + \gamma_B = \alpha_S$: Indeed, in view of Equation (1), we have $D(a|B) - f(a) = ab + \alpha_S - D(b|A) - f(a) = f(b) + \alpha_S - D(b|A)$ for all $a \in A$ and $b \in B$ in this case, implying in particular that neither side changes once we replace a by any other element in A nor b by any other element in B. So, choosing any fixed $a_0 \in A$ and $b_0 \in B$, we may put $\gamma_A := D(a_0|B) - f(a_0)$ and $\gamma_B := D(b_0|A) - f(b_0)$ in which case we have $\gamma_A+\gamma_B = D(a_0|B)+D(b_0|A)-f(a_0)-f(b_0) = D(a_0|B)+D(b_0|A)-a_0b_0 = \alpha_S$, $f(a) = D(a|B) - \gamma_A$ and $f(b) = D(b|A) - \gamma_B$ for all $a \in A$ and $b \in B$. Moreover, we have $\gamma_A \geq 0$ in view of $D(a_0|B) = \frac{1}{2}\min\{a_0b + a_0b' - bb' : b, b' \in B\} = f(a_0) + \frac{1}{2}\min\{f(b) + f(b') - bb' : b, b' \in B\} \geq f(a_0)$, and, similarly, $\gamma_B \geq 0$.

In other words, given any block split $S = A|B$, the set

$$T(D|S) := \{f \in P(D) : E_f \subseteq \binom{A}{2} \cup \binom{B}{2}\}$$

forms an straight line segment in $\mathbb{R}^X$ parametrized by the straight line segment $\{(\gamma_A, \gamma_B) \in \mathbb{R}^2_{\geq 0} : \gamma_A + \gamma_B = \alpha_S\}$ in $\mathbb{R}^2$, and the two end points $f_A := f_{A\to\alpha_S,B\to 0}$ (closer to A) and $f_B := f_{A\to 0,B\to\alpha_S}$ (closer to B) must each be either cut points of $T(D)$ that do not have a neighborhood that is homeomorphic to the open interval $(-1, +1)$ or elements of the set $K(D) := \{k_x : x \in X\}$ consisting of all Kuratowski maps for D. Hence we have the following.

Corollary 2.3 For every block split $S = A|B$ the maps f_A and f_B must be contained in the set $Cut^*(D) := cut^*(D) \cup K(D)$.

3 Key properties of Σ_D and $Cut^*(D)$

As we have seen in the previous section, it is sometimes helpful to consider the bigger set $Cut^*(D)$ rather than $cut^*(D)$. Since we can easily identify

those Kuratowski maps that are not in $cut^*(D)$, we will now focus mainly on $Cut^*(D)$. The following lemma establishes the key properties of Σ_D and $Cut^*(D)$ that we will use in our algorithm to compute these sets recursively.

Lemma 3.1 Let x be an arbitrary element of X. Define $X' := X \setminus \{x\}$ and let D' denote the restriction of D to X'. Then the following assertions hold.

(i) If $S = A|B$ is a block split of X, then either $S = \{x\}|X'$ or the restriction $A \cap X'|B \cap X'$ of S to X' is a block split of X'.

(ii) If $f \in Cut^*(D) \setminus K(D) = cut^*(D) \setminus K(D)$ has the property that there is no block split $S = A|B$ of X with $f \in \{f_A, f_B\}$, then the restriction f' of f to X' is an element of $Cut^*(D')$ and $f(x) = \max\{xy - f'(y) : y \in X'\}$ holds.

Proof: (i) Clearly, if $S = A|B$ is a block split of X with $A, B \neq \{x\}$, then $S' = A \cap X'|B \cap X'$ is a split of X', and there exists a map $f \in P(D)$ such that Γ_f is the disjoint union of two cliques with vertex sets A and B implying that the restriction f' of f to X' is in $P(D')$ and that $\Gamma_{f'}$ is the disjoint union of two cliques with vertex sets $A \cap X'$ and $B \cap X'$, respectively. This establishes (i).

To see that (ii) holds, suppose $f \in cut^*(D) \setminus K(D)$ and that there is no block split $S = A|B$ of X with $f \in \{f_A, f_B\}$. Clearly, the restriction f' of f to X' is in $P(D')$. So, it remains to show that $\Gamma_{f'}$ is disconnected, but not the disjoint union of two cliques, which implies in particular that $f' \in T(D')$.

Assume for a contradiction that $\Gamma_{f'}$ is connected or the disjoint union of two cliques. We first note that this implies that Γ_f has at least one connected component that is a clique. To see this, observe that if $\Gamma_{f'}$ is connected, then Γ_f has precisely two connected components, one of whom consists of the single vertex x, thus trivially forming a clique. Similarly, if $\Gamma_{f'}$ is the disjoint union of two cliques, then one of these cliques is also a connected component of Γ_f.

Let A denote the vertex set of a connected component of Γ_f that forms a clique. Note that this implies that $D(f|A) > 0$. Put $B := X \setminus A$ and $S := A|B$. We want to show that S is a block split with $f \in \{f_A, f_B\}$, yielding the required contradiction. To this end, choose arbitrary elements $a_0 \in A$ and $b_0 \in B$. Since $f \in cut^*(D)$, B cannot be the vertex set of a clique in Γ_f, and so there must exist two distinct elements $b_1, b_2 \in B$ with

the property that $f(b_1) + f(b_2) = b_1 b_2$, implying that $D(f|B) = 0$ holds. Since

$$a'b + ab' = f(a') + f(b) + f(a) + f(b') = a'b' + ab$$

clearly holds for all $a, a' \in A$ and $b, b' \in B$, we have, in view of Equation (1) and the definition of Γ_f,

$$\begin{aligned}\alpha_S &= D(a_0|B) + D(b_0|A) - a_0 b_0 \\ &= (f(a_0) + D(f|B)) + (f(b_0) + D(f|A)) - f(a_0) - f(b_0) \\ &= D(f|A) > 0,\end{aligned}$$

and, therefore, S is indeed a block split.

It remains to show that $f \in \{f_A, f_B\}$. More specifically, we will show that $f = f_B$ holds. By the definition of f_B and in view of the fact that $D(f|B) = 0$ and $D(f|A) = \alpha_S$ holds, we have indeed $f_B(a) = D(a|B) = f(a) + D(f|B) = f(a)$, for every $a \in A$, and $f_B(b) = D(b|A) - \alpha_S = f(b) + D(f|A) - \alpha_S = f(b)$, for every $b \in B$, as claimed. ■

We close this section with establishing bounds on the size of the sets Σ_D and $Cut^*(D)$ that we will use in the analysis of the run time of our algorithm in Section 4.

Lemma 3.2 Let D be a metric on a finite set X with n elements. Then $|\Sigma_D| \leq 2n - 3$ and $|Cut^*(D)| \leq 4n - 5$ holds.

Proof: To establish the first claim, it suffices to note that any two splits $A_1|B_1, A_2|B_2 \in \Sigma_D$ are *compatible*, that is, at least one of the four intersections $A_1 \cap A_2$, $A_1 \cap B_2$, $B_1 \cap A_2$ and $B_1 \cap B_2$ is empty, since it is well known that every set of pairwise compatible splits of X contains at most $2n - 3$ splits (see e.g. Proposition 2.1.3 and Theorem 3.1.4 in [19]). So, assume for a contradiction that there exist two splits $A_1|B_1$ and $A_2|B_2$ in Σ_D that are not compatible. Then we can choose arbitrary elements $a \in A_1 \cap A_2$, $b \in B_1 \cap A_2$, $c \in A_1 \cap B_2$ and $d \in B_1 \cap B_2$. By the definition of a block split, there exist maps $f_i \in T(D)$, $i \in \{1, 2\}$, for which the graph Γ_{f_i} is the disjoint union of two cliques with vertex sets A_i and B_i. But then, by the definition of Γ_{f_1} and Γ_{f_2},

$$\begin{aligned}f_1(a) + f_1(b) + f_1(c) + f_1(d) = ab + cd &< f_2(a) + f_2(b) + f_2(c) + f_2(d) \\ = ac + bd &< f_1(a) + f_1(b) + f_1(c) + f_1(d)\end{aligned}$$

holds, a contradiction.

Next we show $|Cut^*(D)| \leq 4n-5$. Since, clearly, $|K(D)| \leq n$, it suffices to show that $|Cut^*(D) \setminus K(D)| \leq 3n-5$. In [8], it is shown that there exists a block realization $G = G_D$ of D such that the cut vertices in G are in one-to-one correspondence with the elements in $Cut^*(D) \setminus K(D)$. Moreover, the number of cut vertices in any graph is well known to be less than the number of blocks of this graph (see e.g. [12]). Hence, it suffices to show that the number of blocks in G is at most $3n-5$. Yet, it has been shown in [9] that there is a canonical bijection from the set of blocks of G to a set Π of (*strongly*) *compatible* partitions of X, that is, of partitions such that there exist, for any two distinct partitions π_1 and π_2, two necessarily unique subsets $A_1 \in \pi_1$ and $A_2 \in \pi_2$ of X with $A_1 \cup A_2 = X$ (generalizing the concept of compatibility for splits to arbitrary partitions of X). Therefore, it suffices to show that, for all $n \geq 2$, every set of pairwise compatible partitions of X contains at most $3n-5$ partitions which we will establish by induction on the size of X. Clearly, if $n=2$ then there is only one partition of X.

Now assume $n = |X| > 2$. If every partition in Π is a split of X, then $|\Pi| \leq 2n-3 < 3n-5$ must hold. Otherwise, there exists a partition $\pi \in \Pi$ that contains at least three subsets of X. For every $A \in \pi$, fix an arbitrary element $x_A \in X \setminus A$, define Π_A to be the set of the restrictions $\pi'_{|A \cup \{x_A\}}$ of those partitions $\pi' \in \Pi$ with the property that there exists some $A' \in \pi'$ with $A \cup A' = X$, and note that any such partition π' can be recovered from its restriction $\pi'_{|A \cup \{x_A\}}$ as it must consist of all subsets B in that restriction that do not contain x_A and the complement of their union. Thus, it is not hard to see that, for every $A \in \pi$, any two partitions of $A \cup \{x_A\}$ in Π_A are compatible, that $1 + \sum_{A \in \pi} |\Pi_A| = |\Pi|$ holds, and that $|A \cup \{x_A\}| < |X|$ holds for every $A \in \pi$. Hence, by induction,

$$|\Pi| = 1 + \sum_{A \in \pi} |\Pi_A| \leq 1 + \sum_{A \in \pi} (3|A| - 2) \leq 3n - 5,$$

as required. ■

4 The algorithm for computing $Cut^*(D)$

In this section, we present our new algorithm for computing $Cut^*(D)$ called ComputeCutPoints(D) which follows the recursive approach suggested by Lemma 3.1. This algorithm can be regarded as a speed-up of the algorithm

for computing cutpoints presented in [7], which, as mentioned in the introduction, also improves upon the run time of the algorithm presented in [14]. In Figure 2, we present a pseudocode for this algorithm. Besides $Cut^*(D)$ the algorithm returns the set Σ_D and the auxiliary set $\mathcal{A}(\Sigma_D)$, which, for every split $S = A|B \in \Sigma_D$, contains the 4-tuple $(a_S, b_S, D(a_S|B), D(b_S|A))$, where $a_S \in A$ and $b_S \in B$ are fixed elements that are arbitrarily chosen during the course of the algorithm.

To illustrate how our algorithm computes $Cut^*(D)$, consider the metric D presented in Figure 1(a). Suppose in Line 3 of the pseudocode in Figure 2, we select the element c. Consider the restriction D' of D to the subset $X' := X \setminus \{c\}$. A block realization of D' is presented in Figure 1(c). It is easy to check that the set of block splits of D' is

$$\Sigma' = \{\{a\}|\{b, d, e\}, \{b\}|\{a, d, e\}, \{d\}|\{a, b, e\}, \{a, b\}|\{d, e\}\}.$$

Note that the splits in Σ' are in one-to-one correspondence with the edges of the block realization in Figure 1(c). The set $C' := Cut^*(D')$ consists of the Kuratowski maps in $K(D')$ and one additional map $f \in \mathbb{R}^{X'}$ with $f(a) = 2$, $f(b) = 1$, $f(d) = 7$ and $f(e) = 3$. Note that this map corresponds to the cut vertex v in Figure 1(c) as $f(x)$ equals the length of a shortest path from v to x in the block realization for every $x \in X'$.

Given C' and Σ', the algorithm first computes the set Σ of block splits of D and the auxiliary set $\mathcal{A}$ (Lines 6-21). In our example it is easy to check that each of the splits in Σ' gives rise to precisely one split in Σ, that is,

$$\Sigma = \{\{a\}|\{b, c, d, e\}, \{b\}|\{a, c, d, e\}, \{d\}|\{a, b, c, e\}, \{a, b\}|\{c, d, e\}\}.$$

Next the set $C := Cut^*(D)$ is computed (Lines 22-27) by first adding the maps f_A and f_B for every $S = A|B \in \Sigma$. For the metric D in Figure 1(a), this yields, in addition to the Kuratowski maps k_a, k_b and k_d, the 3 cutpoints $(2, 1, 4, 7, 3)$, $(3, 2, 3, 6, 2)$ and $(8, 7, 2, 1, 3)$, where $(x_1, x_2, \ldots, x_5) \in \mathbb{R}^5$ represents the map $f \in \mathbb{R}^X$ with $(x_1, x_2, \ldots, x_5) = (f(a), f(b), \ldots, f(e))$. Note that these cutpoints correspond to the 3 cut vertices in the block realization of D in Figure 1(b). For our example, the computation of C is completed by adding the Kuratowski maps k_c and k_e (Line 27).

Theorem 4.1 Given a metric D on a set X with n elements, the algorithm $\textsc{ComputeCutPoints}(D)$ computes $Cut^*(D)$ in $O(n^3)$ time.

ComputeCutPoints(D)

Input: a metric D on X
Output: $Cut^*(D)$, Σ_D, $\mathcal{A}(\Sigma_D)$

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if $X = \{x\}$, **then return** $C := \{k_x\}$, $\Sigma := \emptyset$ and $\mathcal{A} := \emptyset$.
Initialize $C := \emptyset$, $\Sigma := \emptyset$ and $\mathcal{A} := \emptyset$.
Select $x \in X$ arbitrarily.
Put $X' := X \setminus \{x\}$, and let D' denote the restriction of D to X'.
Compute recursively $C' := Cut^*(D')$, $\Sigma' := \Sigma_{D'}$ and $\mathcal{A}' := \mathcal{A}(\Sigma_{D'})$.
for each $S' = A'|B' \in \Sigma'$ **do**
    Put $a_S := a_{S'}$ and $b_S := b_{S'}$.
    Put $A := A' \cup \{x\}$, $B := B'$ and extend S' to $S := A|B$.
    Compute $D(a_S|B) := D(a_{S'}|B')$.
    Compute $D(b_S|A) := \min\{D(b_{S'}|A'), \frac{1}{2}\min\limits_{a \in A} (b_S x + b_S a - ax)\}$.
    if S is a block split of X, **then**
        Insert S into Σ and $(a_S, b_S, D(a_S|B), D(b_S|A))$ into $\mathcal{A}$.
    Put $A := A'$, $B := B' \cup \{x\}$ and extend S' to $S := A|B$.
    Compute $D(a_S|B) := \min\{D(a_{S'}|B'), \frac{1}{2}\min\limits_{b \in B} (a_S x + a_S b - ax)\}$.
    Compute $D(b_S|A) := D(b_{S'}|A')$.
    if S is a block split of X, **then**
        Insert S into Σ and $(a_S, b_S, D(a_S|B), D(b_S|A))$ into $\mathcal{A}$.
Put $S = \{x\}|X'$, $a_S := x$ and select $b_S \in X'$ arbitrarily.
Compute $D(a_S|X')$ and $D(b_S|\{x\})$.
if S is a block split of X, **then**
    Insert S into Σ and $(a_S, b_S, D(a_S|X'), D(b_S|\{x\}))$ into $\mathcal{A}$.
for each $S = A|B \in \Sigma$ **do**
    Insert f_A and f_B into C.
for each $f' \in C'$ **do**
    Extend f' to $f \in \mathbb{R}^X$ putting $f(x) := \max\{xy - f'(y) : y \in X'\}$.
    if f is a cutpoint of D, **then** insert f into C.
for each $x \in X$ **do** insert k_x into C.
return C, Σ and $\mathcal{A}$.

Figure 2: Pseudocode for our algorithm for computing $Cut^*(D)$.

Proof: We first show that our algorithm is correct. To do this we use induction on the size n of X. Our induction hypothesis is that our algorithm computes $Cut^*(D)$ and the set Σ_D of block splits of X correctly. If $|X| = 1$, there is nothing to prove. Now suppose that $|X| > 1$ holds. Let x be the element in X selected by our algorithm (Line 3), put $X' := X \setminus \{x\}$, and let D' denote the restriction of D to X' (Line 4). By Lemma 3.1(i), the set Σ_D of block splits of X can be computed from the set $\Sigma_{D'}$ of block splits of X'. By induction, the recursive call (Line 5) will correctly compute $\Sigma_{D'}$ and, therefore, our algorithm will correctly compute Σ_D (Lines 6-21). Similarly, by Corollary 2.3 and Lemma 3.1(ii), the set $Cut^*(D)$ can be computed from Σ_D and $Cut^*(D')$. We have argued already that the computation of Σ_D is correct and, again by induction, the recursive call (Line 5) will correctly compute $Cut^*(D')$. Hence, our algorithm will correctly compute $Cut^*(D)$ (Lines 22-27).

We next show that our algorithm has run time $O(n^3)$. We claim that an upper bound $T(n)$ on the run time will satisfy the recurrence $T(n) \leq T(n-1) + O(n^2)$. Using standard techniques for solving recurrences (see e.g. [4]), this yields $T(n) \in O(n^3)$. So, it remains to show that all operations except those performed in the recursive call (Line 5) can be done in $O(n^2)$ time.

We first focus on the computation of Σ_D from $\Sigma_{D'}$ (Lines 6-21). Let $S' = A'|B'$ be an arbitrary split in $\Sigma_{D'}$. We can assume that $D(a_{S'}|B')$ and $D(b_{S'}|A')$ are available from the 4-tuple $(a_{S'}, b_{S'}, D(a_{S'}|B'), D(b_{S'}|A')) \in \mathcal{A}'$. We want to check whether the split $S = A|B = A' \cup \{x\}|B'$ is a block split of X (Line 11). By Lemma 2.2 it suffices to check whether $\alpha_S > 0$ and $a_S b + a b_S = a_S b_S + ab$ holds for all $a \in A$, $b \in B$, using $a_S = a_{S'}$ and $b_S = b_{S'}$. Note that, since S' is a block split of X', it suffices to check whether $a_S b + x b_S = a_S b_S + xb$ holds for all $b \in B$, which can be done in $O(n)$ time. Moreover, since $D(a_S|B) = D(a_{S'}|B')$ and

$$D(b_S|A) = \min\{D(b_{S'}|A'), \frac{1}{2}\min\{b_S x + b_S a - ax : a \in A' \cup \{x\}\}\}$$

hold (Lines 9-10), we can also compute $\alpha_S = D(a_S|B) + D(b_S|A) - a_S b_S$ in $O(n)$ time.

To summarize, whether S is a block split of X or not can be checked in $O(n)$ time. Using completely similar arguments, it can also be shown that checking whether $A'|B' \cup \{x\}$ is a block split of X (Line 16) can be done in $O(n)$ time. Note that, by Lemma 3.2, there are $O(n)$ block splits

of D'. Thus, our algorithm will perform $O(n)$ iterations of the loop in Line 6 and each iteration is completed in $O(n)$ time, yielding $O(n^2)$ in total for Lines 6-17.

To finish the computation of Σ_D, we need to check whether the split $S = \{x\}|X'$ is a block split of X (Lines 18-21). To do this, we fix $a_S = x$ and choose an arbitrary $b_S \in X'$. Then, we compute $D(a_S|X')$ and $D(b_S|\{x\})$, which can be done in $O(n^2)$ time, and check whether $\alpha_S = D(a_S|X') + D(b_S|\{x\}) - a_S b_S > 0$ holds. We also check whether $a_S b + x b_S = a_S b_S + xb$ holds for all $b \in X'$, which can be done in $O(n)$ time. This finishes the analysis of the time needed to compute Σ_D.

Next, we focus on the computation of $Cut^*(D)$ (Lines 22-27). We use a data structure Dic to store the elements in $Cut^*(D)$ computed so far. Since, by Lemma 3.2, $|Cut^*(D)| \in O(n)$, the data structure Dic can be implemented in such a way that inserting a single element of $Cut^*(D)$ into Dic and, later on, checking whether an element of $Cut^*(D)$ has already been stored in Dic both takes $O(n)$ time, see e.g. [11]. Moreover, we assume that, for every $f' \in Cut^*(D')$, the connected components of the graph $\Gamma_{f'}$ have been computed and the cliques among them have been marked.

So, first consider an arbitrary block split $S = A|B \in \Sigma_D$. If we have $A = \{x\}$ and $B = X'$, then we compute f_Y along with the connected components of Γ_{f_Y}, marking the cliques among them, in $O(n^2)$ time for all $Y \in \{A, B\}$. Next we consider the case that there exists some $S' = A'|B' \in \Sigma_{D'}$ such that $A = A' \cup \{x\}$ and $B = B'$ (the following argument is completely analogous if $A = A'$ and $B = B' \cup \{x\}$). Let $a_S \in A'$ and $b_S \in B'$ be the elements that we fixed for S in the course of the algorithm and let $f_{A'}$ and $f_{B'}$ be the maps in $Cut^*(D')$ associated with the split S'. Then we have

$$f_B(a) = D(a|B) = D(a_S|B) - a_S b_S + a b_S = D(a_S|B') - a_S b_S + a b_S = f_{B'}(a)$$

for all $a \in A'$ and

$$f_B(b) = D(b|A) - \alpha_S = a_S b - D(a_S|B) = a_S b - D(a_S|B') = f_{B'}(b)$$

for all $b \in B = B'$, since $D(a_S|B) = D(a_S|B')$ clearly holds. Hence, computing f_B, the connected components of Γ_{f_B} and marking the cliques among them can be done in $O(n)$ time, based on $f_{B'}$ and the connected components of $\Gamma_{f_{B'}}$. Similarly, if $D(b_S|A) = D(b_S|A')$ holds, f_A, the connected components of Γ_{f_A} and the cliques among them can be computed in $O(n)$ time. Otherwise, that is, if $D(b_S|A) < D(b_S|A')$ holds, the graph induced

by Γ_{f_A} on X' is the disjoint union of two cliques with vertex sets A' and B', respectively. To see this, note that $f_A(a) + f_A(a') > f_{A'}(a) + f_{A'}(a') \geq aa'$,

$$\begin{aligned} f_A(b) + f_A(b') &= 2\alpha_S + a_S b + a_S b' - 2D(a_S|B) \\ &> a_S b + a_S b' - 2D(a_S|B') = f_{B'}(b) + f_{B'}(b') \geq bb', \end{aligned}$$

and $f_A(a) + f_A(b) = ab = f_{A'}(a) + f_{A'}(b)$ holds for all $a, a' \in A'$ and $b, b' \in B'$. But then, also in this case, the connected components of Γ_{f_A} and the cliques among them can easily be computed in $O(n)$ time.

It remains to consider an arbitrary $f' \in Cut^*(D')$ (Lines 24-26). Extending f' to f (Line 25), that is, computing $f(x)$ can be done in $O(n)$ time. Recall that we assume that the connected components of the graph $\Gamma_{f'}$ and the cliques among them have been computed. From this information, we can compute in $O(n)$ time the connected components of Γ_f and determine which of them are cliques. Hence the loop in Line 24 will take $O(n^2)$ time, as required. Similarly, the loop in Line 27 will also take $O(n^2)$ time. This finishes the analysis of the run time of our algorithm and thus the proof of the theorem. ∎

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References

[1] H. J. Bandelt and A. Dress. A canonical decomposition theory for metrics on a finite set. *Advances in Mathematics*, 92:47–105, 1992.

[2] D. Bryant and V. Berry. A structered family of clustering and tree construction methods. *Advances in Applied Mathematics*, 27:705–732, 2001.

[3] F. Chung, M. Garrett, R. Graham, and D. Shallcross. Distance realization problems with applications to internet tomography. *Journal of Computer and System Sciences*, 63:432–448, 2001.

[4] T. H. Cormen, C. E. Leiserson, R. L. Rivest, and C. Stein. *Introduction to algorithms*. MIT Press, 2001.

[5] M. Deza and M. Laurent. *Geometry of Cuts and Metrics*. Springer, 1997.

[6] A. Dress. Trees, tight extensions of metric spaces, and the cohomological dimension of certain groups: A note on combinatorial properties of metric spaces. *Advances in Mathematics*, 53:321–402, 1984.

[7] A. Dress, K. T. Huber, J. Koolen, and V. Moulton. An algorithm for computing virtual cut points in finite metric spaces. In *International Conference on Combinatorial Optimization and Applications (COCOA)*, volume 4616 of *LNCS*, pages 4–10. Springer, 2007.

[8] A. Dress, K. T. Huber, J. Koolen, and V. Moulton. Block realizations of finite metrics and the tight-span construction I: the embedding theorem. *Applied Mathematics Letters*, 21:1306–1309, 2008.

[9] A. Dress, K. T. Huber, J. Koolen, and V. Moulton. Compatible decompositions and block realizations of finite metrics. *European Journal of Combinatorics*, 29:1617–1633, 2008.

[10] A. Dress, K. T. Huber, J. Koolen, and V. Moulton. Cut points in metric spaces. *Applied Mathematics Letters*, 21:545–548, 2008.

[11] T. Gonzalez. Simple algorithms for the on-line multidimensional dictionary and related problems. *Algorithmica*, 28:255–267, 2000.

[12] F. Harary and G. Prins. The block-cutpoint-tree of a graph. *Publicationes Mathematicae Debrecen*, 13:103–107, 1966.

[13] A. Hertz and S. Varone. The metric bridge partition problem. *Journal of Classification*, 24:235–249, 2007.

[14] A. Hertz and S. Varone. The metric cutpoint partition problem. *Journal of Classification*, 25:159–175, 2008.

[15] D. Huson and D. Bryant. Application of phylogenetic networks in evolutionary studies. *Molecular Biology and Evolution*, 23:254–267, 2005.

[16] W. Imrich, J. Simoes-Pereira, and C. Zamfirescu. On optimal embeddings of metrics in graphs. *Journal of Combinatorial Theory, Series B*, 36:1–15, 1984.

[17] J. Isbell. Six theorems about metric spaces. *Commentarii Mathematici Helvetici*, 39:65–74, 1964.

[18] C. Kuratowski. Quelques problèmes concernant les espaces métriques non-séperables. *Fundamenta Mathematicae*, 25:534–545, 1935.

[19] C. Semple and M. Steel. *Phylogenetics*. Oxford University Press, 2003.

[20] D. West. *Introduction to graph theory*. Prentice Hall, 1996.